Condensed Matter Physics

A COMPUTATIONAL STUDY OF THE SPECTRUM OF ENDOHEDRAL HYDROGEN AND MAGNESIUM

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In recent years there have been many advancements in our understanding of Fullerene systems due to new methods of Fullerene synthesis. This has lead to the encapsulation of small molecules inside fullerene cages. We investigate the properties of hydrogen-like atoms confined within C_{60} Fullerene. A computer simulation is developed to numerically solve the Schrodinger equation and thus obtain the energy levels of the caged atom or ion. In the simulation, space is divided into finite elements and then using the potential at these locations a Hamiltonian matrix is created. The corresponding eigenvalue problem is then solved numerically to give the electron energy levels and hence the spectrum. The use of symmetry allows the study of atoms in the center of the cage to be modeled as a one-dimensional function, while off center atoms are modeled in two dimensions. The cage potential is approximated using a symmetric square well about the cage radius. A pseudo-potential is used to model the MgII ion, with parameters derived from density-functional theory. We report that most energy states of H are affected little by the confinement. However those states that have an electron with a high probability of being near the cage radius experience a large energy shift. Mg shows similar shifts to those of H. Since the wavefunctions were broader more of the wave functions showed a shift, due to their higher probability of being around the well.